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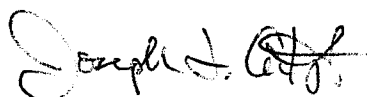
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ABSTRACT

Title: Characterization of a Field-Portable Raman System for Rapid
       Chemical Identification

       Joseph Lawrence Catyb, Master of Science in Public Health, 2007

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Raman spectroscopy is a technology that can be used to rapidly screen unknown chemical substances via direct reading instrumentation. This research focused on the performance of the FirstDefender™, a field-portable Raman spectrometer with a 300 mW 785 nm diode laser and onboard spectral library, by analyzing liquid and solid substances under a variety of conditions. Sixty substances, known to be challenging for Raman spectroscopy, were analyzed in clear glass vials. Eighty-eight percent of substances in the spectral library were correctly or similarly matched with zero false positives. The majority of unmatched substances resulted from fluorescence of white powders. The identification of explosive materials, the effects of different sample containers, and the ability to analyze binary liquid mixtures were also tested. Clear, thin-walled containers did not interfere with the instrument identification accuracy. The importance of having a library with high quality spectra for maximizing instrument accuracy was noted throughout this instrument characterization process.

CHARACTERIZATION OF A FIELD-PORTABLE RAMAN SYSTEM FOR RAPID
CHEMICAL IDENTIFICATION

by

Joseph Lawrence Catyb

Thesis submitted to the Faculty of the Preventive Medicine and Biometrics Graduate
Program of the Uniformed Services University of the Health Sciences in partial
fulfillment of the requirements for the degree of

Master of Science in Public Health

2007

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DEDICATION

- To God for the many blessings that continue to occur in my life.

- To my wife, Lauren, and daughter, Ashley, for their love, patience, and constant encouragement to do my best throughout my military career and this two year academic endeavor.

- To my mother, Gladys, for her love and continued support.

- To my in-laws, Charlie and Judy, because of the help they provided that enabled me to first obtain my bachelor's degree and now an advanced degree.

ACKNOWLEDGEMENTS

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CHAPTER 1

INTRODUCTION

The need for direct reading instrumentation that can quickly and accurately identify unknown substances is critical for homeland defense. Direct reading instruments should be portable, durable, easy to use, as well as, highly sensitive and specific. A direct reading instrument would aid military personnel who are under threat of exposure to chemical or biological warfare agents. Transportation inspection points (i.e. airports) would benefit from instrumentation that could rapidly screen suspect substances and reduce exposures to potentially corrosive or toxic materials. The ability to analyze evidence in forensic investigations without consuming or disturbing evidence would be advantageous. The same would hold true for the analysis of shock-sensitive explosive materials.

One technology that can quickly identify hazardous substances is Raman spectroscopy. The technology was first discovered by Sir C.V. Raman in 1928, but only until recently has Raman spectroscopy moved from the laboratory environment to the field due to advances in optics, lasers, detectors and computing power (Eckenrode, 2001). The use of charge-coupled device array detectors have reduced the measurement time for Raman spectrometers from approximately 10 minutes to only a few seconds in many cases (Bowie, 2000a). Raman is a powerful technique for molecular analysis, capable of identifying organic and inorganic substances in solid, liquid, or gaseous states (Carter, 2005).

Raman spectroscopy is based on the detection of inelastically scattered light from an incident laser source focused onto a sample. The scattered light is shifted in frequency

 due to sample absorbance at frequencies equal to characteristic molecular vibrations (Kneipp, 1999). The resulting spectrum is plotted with intensity as a function of the shifted frequencies in wavenumbers (cm^{-1}). Raman scattering is weak and its intensity is dependent upon several factors displayed in Equation 1.1:

$$I_{Raman} \propto \sigma_v I_{Laser} v_{Laser}^4 \qquad\qquad\qquad \textbf{Equation 1.1}$$

where, I_{Raman} = intensity of bands in a Raman spectrum, σ_v = Raman cross section, typically 10^{-30} to 10^{-25} cm^2/molecule, I_{Laser} = power of the incident laser, and v_{Laser} = frequency of the incident laser. The intensity of Raman scattering is highly dependent on the incident laser frequency and to a lesser degree on the laser power and Raman cross-section for the measured substance.

Raman spectroscopy can be used as a complementary technology to infrared (IR) spectroscopy; however, each process occurs with a different mechanism. IR transitions result from absorption of energy caused by a change in the molecular dipole moment during vibrations (Bartick, 2001). Molecules are Raman-active if a polarizability change occurs during a vibration (Ferraro, 1994). Another distinction between Raman and IR spectroscopy is that the peaks in the Raman spectrum of a material tend to be narrower than those in its corresponding IR spectra (Pearman, 2006). Narrow Raman peaks reduce spectral overlap and can aid in substance identification.

There are several benefits to using Raman spectroscopy for direct reading instrumentation. Substances within transparent or translucent containers can be identified provided the incident laser light can be focused on the substance. Unlike IR, Raman spectroscopy is relatively unaffected by the presence of water, glass and carbon dioxide (Bartick, 2001). Spectral libraries can enable Raman instruments to quickly identify

substances by matching a sample spectrum to an onboard spectrum. Raman spectrometers are amenable to miniaturization for field applications (Eckenrode, 2001). Crime scene evidence can be analyzed without consuming or disturbing material. In most cases, Raman spectroscopy has also been used for the identification of explosive substances in glass and plastic containers (Lewis, 1995).

Several research efforts have focused on the remote use of Raman spectroscopy. In one study, the Raman spectra of 26 explosive materials and 2 plastic explosives were successively collected with a Raman spectrometer equipped with a 10 meter fiber optic probe. The spectra were obtained from samples positioned up to 12 meters from the spectrometer within 4 minutes (Lewis, 2004). A Raman spectrometer with a frequency-doubled 532 nm Nd:YAG pulsed laser and gated intensified charge-coupled device detector was able to detect high explosive materials up to a distance of 50 meters (Carter, 2005). The high explosive samples contained from 4% to 8% of RDX (1,3,5-trinitro-1,3,5-triazacyclohexane) , TNT (2,4,6-trinitrotoluene), PETN (pentaerythritol tetranitrate), and nitrate and chlorate simulants in a dry silica matrix. A Raman spectrometer with a 100 mW 532 nm laser integrated to an unmanned ground vehicle was used remotely to identify a biological agent stimulant (ovalbumin) on a flat sheet of galvanized iron duct material (Gardner, 2007).

Raman spectroscopy also has some limitations. Harvey *et al*. (2003) found that a near-infrared (NIR) 785 nm diode laser operating at 300 mW is sufficient to heat and possibly burn samples, particularly if the laser radiation is absorbed rather than scattered. Darker colors have the highest propensity for sample heating (Harvey, 2003). In addition, heating can change the structure of a sample resulting in shifting Raman peaks

and creation of new peaks (Bowie, 2000b; Vickers, 1992). As a result, sensitivity is

compromised because the Raman scattering cross-section is reduced, so low level trace

identification is difficult with traditional Raman (Stuart, 2006; Knözinger, 1999).

However, research is being conducted with another Raman technique, surface-enhanced

Raman spectroscopy (SERS), which has identified trace amounts of toxin simulants, and

biological and chemical warfare agents and simulants, including vapor phase detection

(Farquharson, 2005; Pearman, 2006; Stuart, 2006).

Fluorescence is also a problem that can interfere with the interpretation of Raman

spectral data. Fluorescence is generally described as sample-generated emitted light that

can dominate a Raman spectrum and will likely occur if the laser wavelength corresponds

to the energy required for transition to an electronic state for either the sample or an

impurity (Bowie, 2000b). Though not limited to these substances, fluorescence has been

commonly encountered when analyzing explosives and white powders (Farquharson,

2003; Lewis, 2004). Fluorescence can be minimized by using lasers that emit energy at

higher wavelengths; however, higher wavelength lasers can reduce Raman signal and

potentially compromise detection. NIR excitation sources such as 785 and 840 nm diode

lasers and the 1064 nm Nd:YAG laser are popular choices for Raman spectrometers

because fewer compounds have electronic energy states that correspond to an NIR

wavelength (Bowie, 2000a). Mathematical techniques such as principal component

analysis and polynomial curve fitting have also been used to separate Raman spectra

from fluorescence (Hasegawa, 2000; Lieber, 2003). Baseline correction to remove the

elevated baseline caused by fluorescence is a commonly used technique (Bowie, 2000b).

However, fluorescence continues to be problematic for Raman spectroscopy.

The purpose of this research was to evaluate the performance of the First Defender™ hand-held portable Raman spectrometer (Ahura Scientific, Wilmington, MA) as a chemical screening and classification tool for solid and liquid substances. The FirstDefender™ weighs four pounds, is chemically-resistant, self-contained and uses a NIR 785 nm diode laser as the incident light source. The FirstDefender™ uses a spectral library to match sample Raman spectra and contains proprietary software to deconvolute chemical mixtures.

A previous evaluation of the FirstDefender™ resulted in identifying 32 of 33 substances (97%) present in the spectral library (Eckenrode, 2006). The substances, consisting of pure chemicals, commercial compounds and biologically-derived compounds, were evaluated in 2 mL clear glass vials using the instrument's vial mode of analysis. Zero false positive results were obtained for substances present in the spectral library.

In testing performed at the U.S. Army Edgewood Chemical and Biological Center, the FirstDefender™ was used to identify chemical warfare agents mixed with several interferents (Matthews, 2006). Distilled mustard (HD), nitrogen mustard (HN3), lewisite (L), and the nerve agents VX, tabun (GA), sarin (GB) and soman (GD) were mixed in sealed glass vials with the following substances in concentrations ranging from 1.25% to 66% (v/v): JP8 jet fuel, aqueous film forming foam (AFFF), floor wax, and glass cleaner. Spectra were collected for the pure chemical warfare agents and interferents and then user-added to the onboard library. Fifty-seven of 66 analyses (86%) resulted in correct identification of the chemical warfare agent. Analysis of the following samples failed: VX in 1.25% to 10% of glass cleaner (4 analyses), VX in 25% of AFFF,

GA in 3.125% and 6.25% of glass cleaner (2 analyses), GA in 12.5% of floor wax, and L in 25% of JP8.

Research Question: Four specific aims will be used to answer the following research question: do white powders, packaging materials, and binary liquid mixtures affect the identification capabilities of the FirstDefender™?

Specific Aims:

1. Analyze 60 substances, known to be challenging to Raman spectroscopy, to include pure chemicals, commercial products, acids, bases, chemical agent simulants and biological/biologically-derived substances to test the instrument's ability to correctly identify the substance.

2. Evaluate the effect of 10 different sample containers on instrument identification accuracy by analyzing six substances known to produce good Raman spectra.

3. Evaluate the identification capability against increasing material thickness of two different materials using four chemical substances.

4. Test instrument's capability to identify explosive materials, and liquid binary mixtures of chemicals and chemical warfare simulants at varying concentrations. Pure chemicals and field samples will be used for explosive material identification. Four binary mixtures will be prepared at three concentrations (1%, 5%, 10% v/v).

Characterization of a Field-Portable Raman System for Rapid Chemical Identification

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Abstract

Raman spectroscopy is a technology that can be used to rapidly screen unknown chemical substances via direct reading instrumentation. This research focused on the performance of the FirstDefender™, a field-portable Raman spectrometer with a 300 mW 785 nm diode laser and onboard spectral library, by analyzing liquid and solid substances under a variety of conditions. Sixty substances, known to be challenging for Raman spectroscopy, were analyzed in clear glass vials. Eighty-eight percent of substances in the spectral library were correctly or similarly matched with zero false positives. The majority of unmatched substances resulted from fluorescence of white powders. The identification of explosive materials, the effects of different sample containers, and the ability to analyze binary liquid mixtures were also tested. Clear, thin-walled containers did not interfere with the instrument identification accuracy. The importance of having a library with high quality spectra for maximizing instrument accuracy was noted throughout this instrument characterization process. It was also found that dark colored

substances could ignite using the 300 mW power setting that was selected for all of the

analyses in this evaluation.

This manuscript has been completed in partial fulfillment of the degree of Master of Science in Public Health, Department of Preventive Medicine and Biometrics, Uniformed Services University of the Health Sciences, Bethesda, Maryland. The opinions or assertions contained herein are the private ones of the authors and are not to be construed as official or reflecting the views of the United States Department of Defense, Uniformed Services University of the Health Sciences, or the Federal Bureau of Investigation.

INTRODUCTION

The potential use of hazardous materials in spreading terror among civilian populations and inflicting casualties in military conflicts has heightened awareness in the post-9/11 era. Law enforcement, military and civilian first responders have a critical need to quickly and accurately identify unknown materials with rugged, field-portable, direct reading instrumentation. It is highly desirable to analyze potentially hazardous materials, chemical agents, and explosive substances within containers to reduce the risk of exposure to personnel and preserve evidence.

A developing technology for direct reading, field-portable instrumentation capable of identifying unknown substances relies on vibrational spectroscopy. Two types of applications using vibrational spectroscopy are infrared (IR) and Raman spectrometry. With IR, a molecule absorbs radiation from the IR source at frequencies that initiate vibrational transitions from lower to higher energy states. The energy absorbed induces vibrations within the molecule such as symmetric and asymmetric bending and stretching. Spectral data can then be used to analyze the relationship between the absorption intensity versus the frequency absorbed for a specific molecule. Water and carbon dioxide strongly absorb IR which can interfere with the spectrum for a substance of interest.

Raman spectroscopy was discovered in 1928 by the Indian physicist, Sir C.V. Raman (Ferraro, 1994). Raman spectroscopy relies on the principle of detecting scattered light from an incident laser source. Most of the photons are scattered elastically (Rayleigh scatter), but a small fraction is inelastically scattered (Raman scatter) (Ingle, 1988). With elastic scattering, energy is absorbed by a molecule at the incident laser's

frequency (ν_0) and subsequently emitted at the same frequency. Inelastic scattered

energy is produced when the incident radiation interacts with the molecule during one of

its vibrational modes at a given frequency (ν_V). With inelastic scatter, the molecule

absorbs energy from the incident source at ν_0 but the emitted or scattered energy is

shifted in frequency by $\pm \nu_V$. A negative shift, $\nu_0 - \nu_V$, is referred to as Stokes scatter

and a positive shift, $\nu_0 + \nu_V$, as anti-Stokes scatter (see Figure 2.1). Multiple shifts in

frequency (ν_V) for a molecule may exist because different bonds will vibrate at different

frequencies. The peaks in Figure 2.1 correspond to symmetric vibrations (459 cm^{-1}) and

asymmetric vibrations (218 and 314 cm^{-1}) occurring within the carbon tetrachloride

(CCl_4) molecule. Consequently, Raman spectra can be used to deduce molecular

structural components.
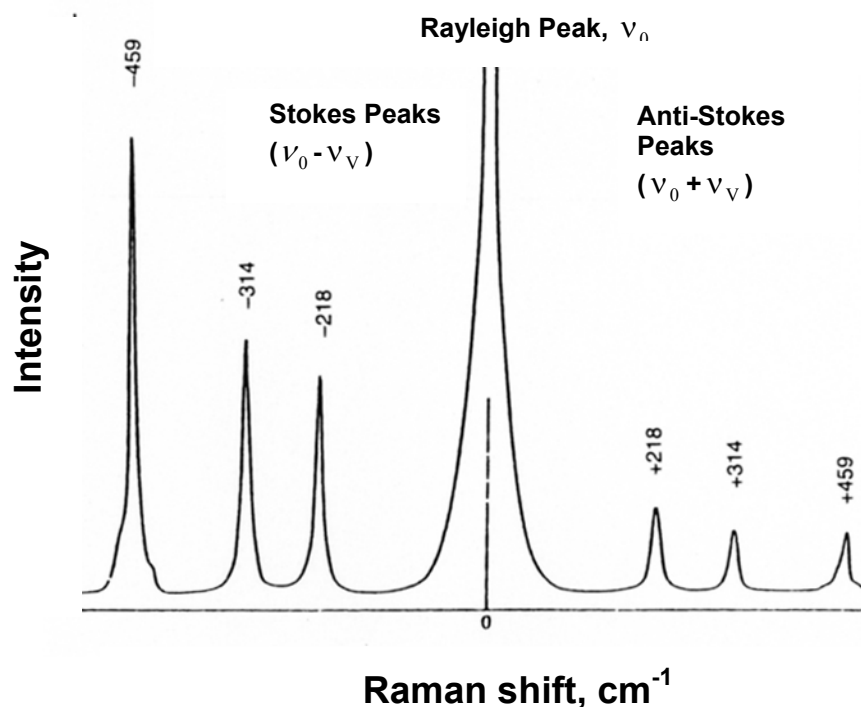
Figure 2.1. **Illustration of Raman and Rayleigh scattering for CCl$_4$**

Raman signals are much smaller than Rayleigh scattered signals. Because of this, the Rayleigh scattered light is usually removed with notch filters and does not appear in the final spectrum (Bowie, 2000a). Also, anti-Stokes scatter is usually not present in the final spectrum since the Stokes scatter is more dominant.

Raman spectroscopy has several advantages over IR. Samples can be analyzed without interference from water or carbon dioxide absorption (Bartick, 2001). Samples can be identified through translucent or transparent containers (i.e. plastic or glass). Properties of the laser source makes it relatively easy to interrogate surfaces, films, powders, solutions, gases and many other sample types (Eckenrode, 2001).

While Raman spectroscopy has demonstrated many positive characteristics, some limitations are exhibited. The incident laser source can be destructive, especially at high power levels. Dark-colored materials/substances will absorb the energy and the substances may ignite (Harvey, 2003). If fluorescence occurs, as is common with white powders, strong and broad bands are generated that can obscure the Raman signal. Fluorescence is the result of a molecule being excited to an electronic energy level, and then reemitting the energy as light at a longer wavelength upon relaxation to a ground energy state. Positive identification of a substance with Raman spectroscopy is dependent on whether the substance is present in the instrument's spectral library. Additionally, mixtures can present a problem if there is not a match to the mixture or to a specific chemical in the spectral library. Algorithms can help to resolve mixtures depending on complexity.

Recent advances in optics, lasers, detectors and other instrument components have contributed to an increased interest in Raman spectroscopy for field chemical

identification (Eckenrode, 2001). Raman spectroscopy has been demonstrated to remotely identify samples at distances up to 50 meters (Carter, 2005; Lewis, 2004; Sharma, 2005). A robot-based Raman spectrometer attached to an unmanned ground vehicle has been developed for identification of chemical, biological and explosive threat agents (Gardner, 2007).

The purpose of this research was to evaluate the performance of the First Defender™ hand-held portable Raman spectrometer (Ahura Scientific, Wilmington, MA) as a chemical identification tool. This research was designed to evaluate accuracy of the FirstDefender™ against a selection of substances such as pure chemicals, commercial products, explosives materials, and biologically-derived substances. In addition, the effects of packaging materials and the ability to identify various chemicals in a mixture were tested.

MATERIALS AND METHODS

Raman spectrometer

The FirstDefender™ (see Figure 2.2) is a ruggedized unit designed for rapid field identification of unknown chemicals. The unit weighs approximately 4 pounds, measures 12 in x 6 in x 3 in, and can operate from either a rechargeable 5-hour battery pack or an AC adaptor. A diode laser (785 ± 0.5 nm), with adjustable power settings of 50, 100 and 300 mW, is used as the incident energy source. The spectral range is 250 to 2875 cm^{-1} and the maximum spectral resolution is 7 to 10 cm^{-1}.

Figure 2.2. Ahura Scientific FirstDefender™ Raman Spectrometer (Courtesy of Ahura Scientific)

The instrument can be operated in two scanning configuration modes: vial and point-and-shoot. In vial mode, samples collected in a vial can be placed into an enclosed compartment for measurement. Samples can also be analyzed in the point-and-shoot mode where a detachable nose cone is pointed at the substance to be scanned. The nose cone can be adjusted such that the focal point of the laser:

- is approximately 0.078 in (78 mils) beyond the tip (nose cone out)
- approximately 0.25 in (250 mils) beyond the tip (nose cone in)
- approximately 0.75 in (750 mils) from the laser aperture (nose cone removed)

The focal point of a laser is the most intense area of the beam and will generate the best Raman signal when it interacts with the substance of interest. The manufacturer recommends nose cone adjustment depending upon the physical state (solid versus liquid) and whether the measured substance is free-standing (e.g. a pile or puddle) or housed in thin (<0.125 in or 125 mils thick) or thick-walled containers. Nose cone removal is suggested when scanning thick-walled containers.

The FirstDefender™ was used in accordance with the manufacturer's guidance. Data were collected using the instrument's fully-automatic mode with spectral library version 64, which contains 2151 substances. A proprietary software package is employed

with the spectral library to generate sample analysis results. The results are displayed as one of the following:

- Positive match to one or more library spectra
- A chemical mixture
- No match found to any library spectra

If the measured Raman spectrum of a scanned substance can be matched to a substance in the spectral library, the result will be a single match or a list of several potential matches. If several matches are displayed, each match is assigned a percentage which corresponds to a probability indicating how well the measured Raman spectrum corresponds to one library spectrum over another.

If the measured Raman spectrum cannot be matched to any of the library spectra, the instrument performs a mixture analysis using a combination of library spectra to match the sample spectra. The result would then be displayed as "Mixture" followed by a list of two or more substances from the spectral library with percentages indicating the amount of Raman spectrum attributed to each substance. It is important to note that the percentages displayed are not proportional to concentration.

The instrument may calculate that the measured spectrum does not match any substance in the spectral library. If a corresponding match is not found in the spectral library, the instrument may still display substances whose spectra exhibit similar features to the sample analyzed.

Sample analysis in this research was conducted in a controlled setting with standard room fluorescent lighting and an ambient temperature of 20-25ºC. Triplicate scans were performed for the analysis of most substances. In some cases, four or more scans were performed if the optimal nose cone position for a testing configuration was

unknown. Scans were generally aborted if the analysis time exceeded three minutes or fluorescence overwhelmed the Raman signal. Some scans were allowed to exceed 3 minutes if the Raman signal continued to increase.   All data were collected in the automatic mode and the laser power was set at 300 mW for all scans. The GRAMS/AI software application was used to examine select spectra when a match was not found.

Vial and Point-and-Shoot Analyses

To evaluate the instrument's ability to collect quality spectra, 60 known samples (exemplars) in 2 mL clear glass vials (Sigma Aldrich, St. Louis, MO) were analyzed in both vial and point-and-shoot modes. The exemplars consisted of pure substances, commercial products, acids and bases, chemical warfare agent simulants, and biologically-derived substances, most of which were problematic for analysis by Raman spectroscopy in previous evaluations. Forty-six white powders, 9 clear liquids, and 5 powders of various colors were analyzed. Of the 60 substances, 36 had corresponding library spectra and 24 were not in the library. The vials were filled with a few milligrams of material such that the focal point of the laser could be oriented to generate the optimal Raman signal.

For vial mode scans, each vial was inserted into the instrument's enclosed compartment for analysis, using a protective lid to block out ambient light. For point-and-shoot mode scans, the height of a styrofoam block containing the vial was adjusted to align the nose cone tip with the vial. The configuration provided consistent distance and orientation for each scan. Each vial was wiped with an isopropyl alcohol swab prior to analysis and also rotated approximately ¼ turn between scans in each mode. Per

manufacturer's guidelines, data were primarily collected with the focal point

approximately 0.25 in (250 mils) beyond the nose cone tip for liquids (nose cone in) and

approximately 0.078 in (78 mils) beyond the tip for solids in thin-walled containers (nose

cone out).

Packaging Material and Container Effects

To evaluate the effect various containers have on instrument response, six pure

substances (4 solid and 2 liquid) known to produce good Raman spectra were placed into

the following containers:

- KAPAK® bag (8 in x 12 in, 4.5 mils)
- Bitran® bag (9 in x 12 in, 3.0 mils)
- ALOKSAK® bag (5 in x 4 in, 6.0 mils)
- 15 mL Falcon™ tube (polystyrene, 32 mils wall thickness)
- 50 mL Falcon™ tube (polypropylene, 38 mils wall thickness)
- 1.2 mL Corning cryovial (polypropylene, 57 mils wall thickness)
- 500 mL polyethylene bottle (53 mils)
- 2 mL amber glass vials (Sigma Aldrich, 38 mils)
- Green glass wine bottle (105 mils)
- Green glass soda bottle (97 mils)

Material thicknesses were obtained for the KAPAK®, Bitran®, and ALOKSAK® bags, the

polyethylene (PE) bottle, the amber glass vial, and the green glass containers using a

micrometer graduated to 0.001 in (Starrett Micrometer No. 216). Manufacturer's data

were used to obtain thicknesses for the Falcon™ tubes and the cryovial. Manufacturer's

guidelines were followed with the focal point approximately 0.25 in (250 mils) beyond

the nose cone tip for scans of the bags and amber vial (nose cone in). Scans of the thicker

green glass bottles were performed with and without the nose cone. The nose cone

position was varied for scans of the tubes, cryovial and PE bottle since it was not known

how the thickness of those materials would affect results.

Influence of Material Thicknesses

The influence of material thickness on correct identification was tested using the KAPAK® and ALOKSAK® bags containing one of four chemicals: ammonium perchlorate, potassium nitrate, sodium bicarbonate and potassium chlorate. KAPAK® bags have a slightly opaque quality whereas the ALOKSAK® bags are transparent. Bag thickness was increased by cutting the bags into square sections and placing multiple layers over the portion of the bag containing the chemical. The bag was laid flat onto an anti-static mat and taped down. Successive layers were then placed over the bag and the edges tightly secured with packaging tape. Scans with the KAPAK® bag were collected at thicknesses of 14, 23, 32, 59 and 77 mils. Scans with the ALOKSAK® bags were collected at thicknesses of 18, 30, 42, 78 and 114 mils. All material thickness scans were performed with the focal point 0.25 in (250 mils) beyond the nose cone tip, which was placed in the center of the squared section.

Influence of Chemical Concentration

The instrument was presented with 1%, 5%, and 10% (v/v) concentrations of the following three analyte-solvent pairings to assess the capability of identifying the analyte in a binary liquid mixture:

- Isopropanol (70% commercial brand) in water (0.1 μm filtered molecular biology reagent, Aldrich Chemical Co.)
- Ethanol (HPLC grade, Acros, CAS 64-17-5) in water (0.1 μm filtered molecular biology reagent, Aldrich Chemical Co.)
- Dimethyl methylphosphonate or DMMP (97%, Aldrich Chemical Co., CAS 756-79-6) in water (0.1 μm filtered molecular biology reagent, Aldrich Chemical Co.)

Approximately 1 mL of each solution was added to a 2 mL clear glass vial (Sigma Aldrich, St. Louis, MO) and capped. Analysis was performed within two minutes of mixing. The vials were wiped with an isopropyl alcohol swab prior to insertion into the vial compartment and rotated approximately ¼ turn between scans. Triplicate scans were performed for each concentration.

Explosive Materials

Fifteen samples were evaluated to assess identification capability of explosive materials. Thirteen forensic field samples containing RDX and two lab-prepared samples containing PETN were tested. The RDX samples were solid materials stored in 4 mL amber glass vials. Preliminary scans confirmed that amber vials did not interfere with spectral in vial mode. Solid PETN (>99% purity) was obtained from the FBI Explosives Unit of the Laboratory Division (Quantico, VA) and added to a 2 mL clear glass vial and scanned in vial mode for one of the PETN samples. A 1000 ppm solution of PETN in methanol (HPLC Grade, Fisher Scientific, Fair Lawn, NJ) was analyzed in vial mode for the second PETN sample.

Scanning of Uncontained Material

Free-standing substances were analyzed in point-and-shoot mode to simulate a field situation where a substance should remain undisturbed. Four pure substances (ammonium perchlorate, potassium nitrate, sodium bicarbonate, potassium chlorate) and two commercial products (baby powder, corn starch) were evaluated by placing

approximately 0.5 in^3 of each substance in a small pile on a sheet of white paper. The

nose cone tip was used to guide placement of the focal point into the substance.

RESULTS AND DISCUSSION

Results from analyses were grouped into one of these five categories:

- Match = an exact match or the highest percentage component in a list of

  matches or a mixture

- Similar Match = a match to a similar substance by chemical class (e.g. lead

  nitrate for silver nitrate) or by type of substance (e.g. corn starch for flour)

- No Match Found (NMF) = result as reported by the instrument

- False Positive = a result for a completely different chemical either as an

  exact match or the highest percentage component in a list or mixture

- Aborted Scan = the analysis time exceeded 3 minutes and generated little to

  no Raman signal

The most repeated result for replicate analysis of the same substance was taken as

Analysis Mode/Type	Number of Spectra Collected	Aborted Scans
Vial Mode	159	22
Point-and-Shoot Mode	167	26
Packaging Materials/Containers	89	10
Material Thicknesses	117	3
Chemical Concentrations	18	9
Explosive Materials	39	3
Uncontained Material	15	3
Total	604	76

Table 2.1. Number of Spectra and Aborted Scans Generated

the representative result for the substance. A total of 680 analyses were performed producing 604 spectra and 76 aborted scans (see Table 2.1). Most of the aborted scans were due to the analyses of substances not in the spectral library, which is a preferred result over an incorrect identification.

Vial and Point-and-Shoot Analyses

Results for substances in the library had favorable correct match percentages with zero false positive readings. Of the 36 substances analyzed with corresponding library spectra, 30 (83%) were correctly or similarly matched in vial mode and 33 (92%) were correctly or similarly matched in point-and-shoot mode (see Table 2.2). Twenty-five of the 60 substances were pure chemicals, of which 24 matched correctly in both modes. The only unmatched pure chemical was white granular oxalic acid. Raman analysis of oxalic acid resulted in an NMF that was most likely due to the fluorescence observed. Only 1 of 7 commercial substances analyzed in vial mode and 2 of 7 in point-and-shoot mode had correct matches; however, all were white powders that are prone to

Result	# of Substances Analyzed in Vial Mode		# of Substances Analyzed in Point-and-Shoot Mode	
	In Library	Not In Library	In Library	Not In Library
Match	28 (77%)	0	30 (83%)	0
Similar Match	2 (6%)	8 (33%)	3 (8%)	8 (33%)
No Match Found	4 (11%)	9 (37%)	2 (6%)	9 (37%)
False Positive	0	3 (13%)	0	3 (13%)
Aborted Scan	2 (6%)	4 (17%)	1 (3%)	4 (17%)
Total	36	24	36	24

Table 2.2. Results for Vial and Point-and-Shoot Analyses

fluorescence.

For the 24 substances without a corresponding spectra in the library, the primary concern was for an incorrect match (i.e. false positive) in which the instrument mistakenly matched the sample to a substance in the spectral library. Ideally, the analysis of a substance without a corresponding spectrum in the library would result in NMF. This was the result for 9 of the 24 (37%) substances analyzed in both vial and point-and-shoot modes. However, 3 of the 24 (13%) non-library substances analyzed (boric acid, strontium sulfate and a commercial non-dairy creamer) resulted in false positives in both modes. False positive results are likely to decrease as quality spectra are added to the instrument's spectral library.

Results for chemical warfare agent surrogates, DMMP and DIMP (diisopropyl methylphosphonate), were acquired by the instrument within 30 seconds. While DMMP was correctly matched correctly, DIMP was identified as Sarin (categorized as a Similar Match) because there was no corresponding library spectrum for DIMP. This illustrates that identifying dangerous chemicals is possible through clear containers without endangering human health.

Packaging Material and Container Effects

Nose cone position is critical to insure that the laser focal point is interacting with the target substance and not the container or packaging material. Recall that the focal point distance relative to the nose cone tip or the laser aperture varies based on nose cone position:

- 0.078 in (78 mils) – nose cone out
- 0.25 in (250 mils) - nose cone in

- 0.75 in (750 mils) - nose cone is removed

Table 2.3 values indicate the number of correct matches out of 3 analyses for each material-substance pair. Most of the substances were correctly matched for the materials and containers with the exception of 3% hydrogen peroxide. No matches were obtained for 3% hydrogen peroxide in the cryovial and green glass bottles. Analysis in the 1.2 mL cryovial resulted in a match to polypropylene, the cryovial's primary component. The minimum laser focal point distance (78 mils) is greater than the cryovial's wall thickness of 57 mils; however, the polypropylene match indicates that the cryovial material produced Raman scatter and likely attenuated the laser such that the weak Raman signal of 3% hydrogen peroxide was overwhelmed by the Raman signal for polypropylene. All six analyses with 3% hydrogen peroxide in the green glass bottles

Packaging Material or Container Type	Thickness, mils	3% Hydrogen Peroxide	70% Isopropanol	Ammonium perchlorate	Potassium nitrate	Sodium bicarbonate	Potassium chlorate
50 mL Falcon™ tube[1]	38	3	3	3	3		
15 mL Falcon™ tube[1]	32	2	3	2	2		
1.2 mL cryovial[1]	57	0	2	2	2		
500 mL PE bottle[1]	53	3	3				
Green soda bottle	97	0	2				
Green wine bottle	105	0	3				
2 mL amber glass vial	38	2	3				
KAPAK® bag[1]	4.5			3	3	3	3
Bitran® bag[1]	3			3	3	3	3
ALOKSAK® bag[1]	6			3	3	3	3

[1]Used by the FBI to collect evidence

Table 2.3. Number of Correct Matches for Packaging Material/Container and Substance Pairings (n=3).
Note: Grayed cell indicates which pairings were not analyzed.

were aborted. Most likely, the Raman signal generated from the hydrogen peroxide was also too weak to overcome any effects from the thicker colored glass. This occurred despite removal of the nose cone to insure the focal point was positioned in the sample versus the glass. Two of three analyses in the amber glass vials resulted in matches for 3% hydrogen peroxide, but only after scan times exceeded 4 minutes. No delay was observed during the vial mode analysis of 3% hydrogen peroxide in a clear glass vial of similar thickness, which suggests the amber color resulted in a weak Raman signal for hydrogen peroxide.

Higher concentrations of the target substance were more easily matched with the colored glassware. Isopropanol (70% in water) was correctly matched in all 3 colored glass containers for 8 of 9 analyses. Reduced analysis times and spectra of lower fluorescence were obtained for the isopropanol samples in the green wine and soda bottles after the nose cone was removed. Removal of the nose cone permitted the laser to fully penetrate the glass and positioned the focal point into the isopropanol, thereby generating a stronger Raman signal for identification. These results confirm that transparent or translucent, thin-walled containers generally do not interfere with Raman identification if the substance yields a strong Raman signal.

Influence of Material Thicknesses

Figure 2.3 displays the percentage of substances that were correctly matched at various thicknesses. All analyses were conducted with the focal point approximately 0.25 in (250 mils) beyond the nose cone tip which was greater than the highest thickness
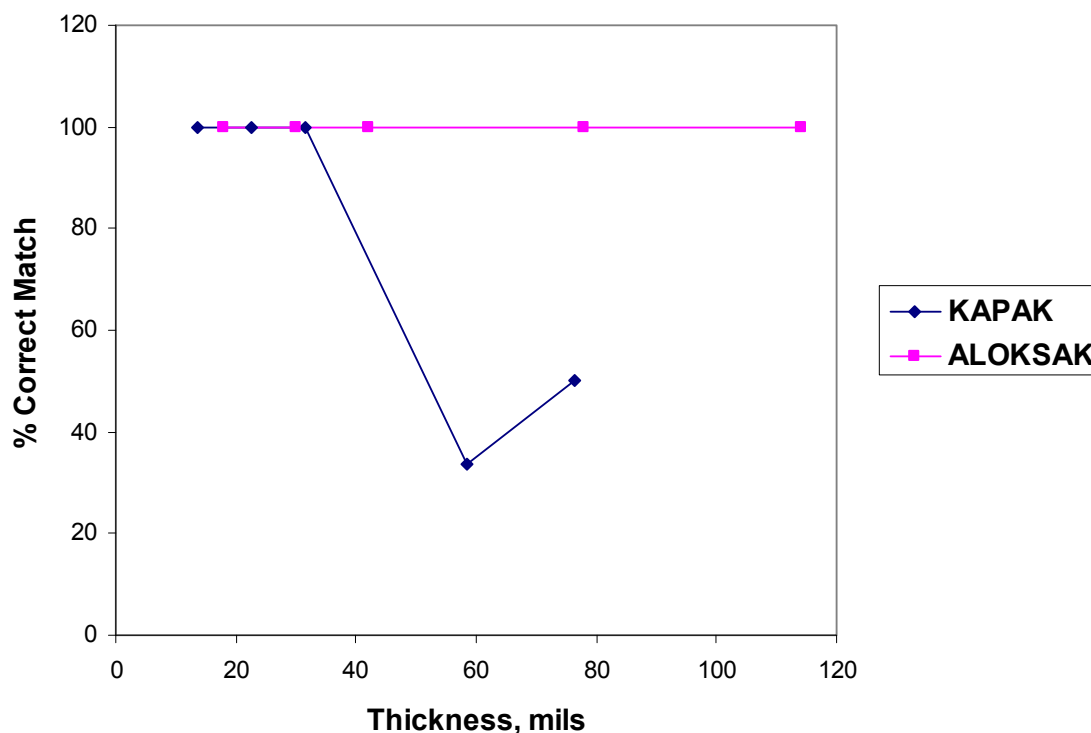
Figure 2.3. **Percent of Substances Correctly Matched versus Thickness for KAPAK and ALOKSAK Bags**

evaluated (114 mils). Material thickness influenced results with the KAPAK[®] bag but

not with the ALOKSAK[®] bag. Results for the KAPAK[®] bags transitioned from an exact

match to NMF and mixtures at a thickness of 58.5 mils for all 4 substances analyzed.

Analysis of an empty KAPAK[®] bag displayed several prominent spectral peaks that were

present in the KAPAK[®] bag analyses of 58.5 and 76.5 mils which most likely

overwhelmed the Raman signal generated from the sample. The slightly opaque

appearance of the KAPAK[®] bags likely led to the degradation in results at 58.5 mils.

Analysis of samples in the clear ALOKSAK[®] bags resulted in correct matches for all

scans in bag thickness up to 114 mils.

Influence of Chemical Concentration

The FirstDefender™ was successful in identifying the solute in 2 of 3 binary

liquid mixtures at 5% and 10% concentrations. Table 2.4 summarizes the number of

analyses that yielded correct or similar matches for each solute-solvent pair. All 1%

solutions resulted in aborted scans which is consistent with the fact that Raman

spectroscopy is not known as a trace technique (Eckenrode, 2001; Pearman, 2006). Both

the 5% and 10% isopropanol (70% in water) and water mixtures consistently matched to

a commercial white board cleaner spectrum from the instrument's spectral library, which

was considered a similar match since it contained isopropanol. Ethanol was the dominant

component in 2 of 3 analyses for the 10% ethanol/water mixture. An interesting result

occurred on the third analysis of the 10% ethanol/water mixture. The instrument reported

a missing percentage of 66% and a match for ethanol at 28%. This was interpreted as a

similar match because the "missing" result could not be matched to anything in the

spectral library by the current algorithm.

		Correct Match of 3 Replicates per Concentration (v/v)		
Solute	Solvent	1%	5%	10%
Isopropanol (70% in water)	Water	0	3	3
Ethanol	Water	0	1	3
DMMP	Water	0	0	0

Table 2.4. Number of Analyses Yielding a Match or Similar Match for Solute

For DMMP/water mixture, 4 of the 6 scans at 5% and 10% concentrations did list

DMMP at a low probability. The results showed DMMP with 2-21% match as the

second choice to bleach. There were common spectral features between bleach and

DMMP at 230, 714, and 1340 cm^{-1} which likely caused the algorithm to match strongly

to the library spectrum for bleach versus DMMP (see Figure 2.4).

While the FirstDefender™ did not identify the DMMP/water mixtures, it is likely

that various concentrations of a DMMP/water mixture could be detected if a spectrum of

10% DMMP/water was added to the spectral library.
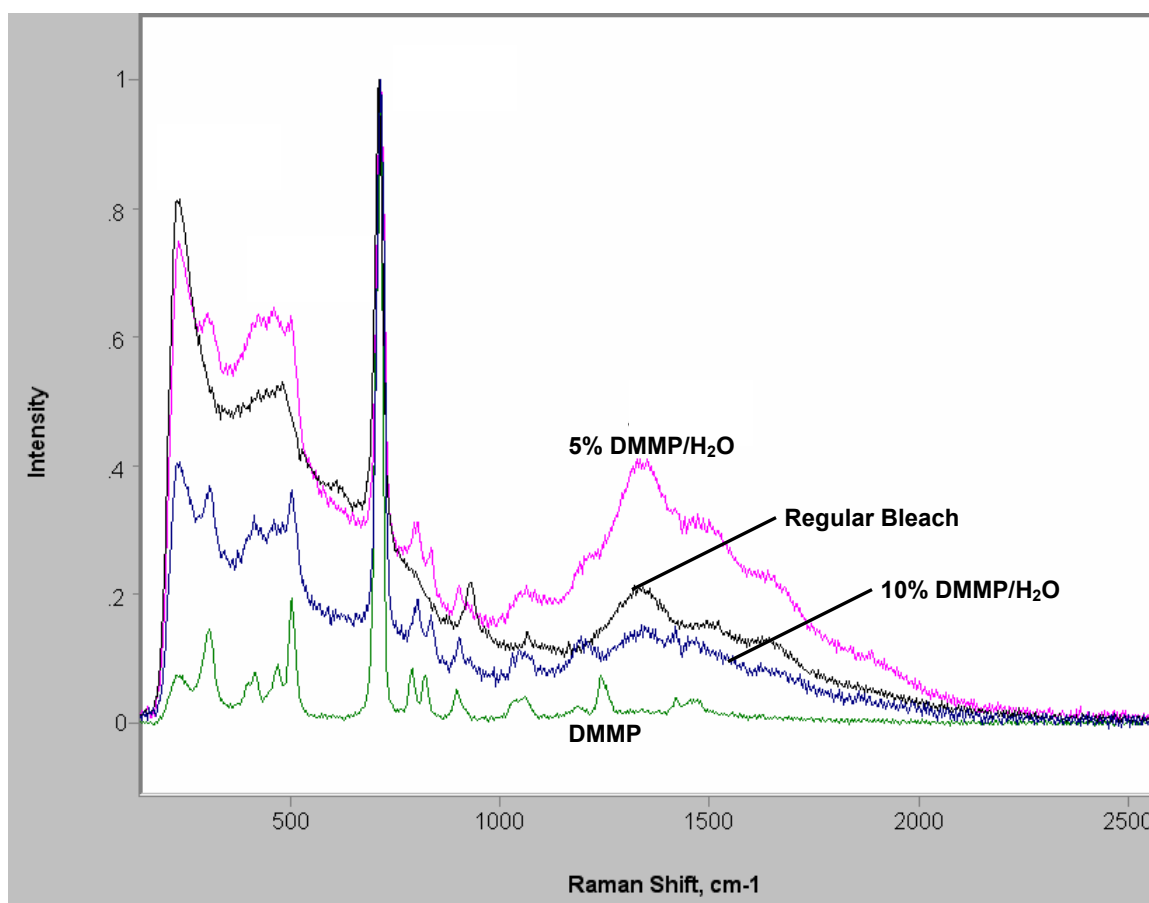
Figure 2.4. Spectral Overlay of DMMP/H₂O Results with Regular Household Bleach

Explosive Materials

No correct matches were obtained for the 13 field forensic samples that contained RDX. After discussions with Ahura scientists, it was determined that the RDX spectrum in library version 64 was a spectrum for an RDX and HMX (1,3,5,7-tetranitro-1,3,5,7-tetra-azacyclooctane) combination and the percentage of each was unknown. One of the unmatched spectra was sent to Ahura and reanalyzed against an upgraded spectral library (version 65, containing 3100 substances) containing a spectrum for pure RDX. The analysis resulted in a correct match for RDX. Figure 2.5 shows the pure RDX library spectrum overlaid with the spectrum from the field forensic sample.
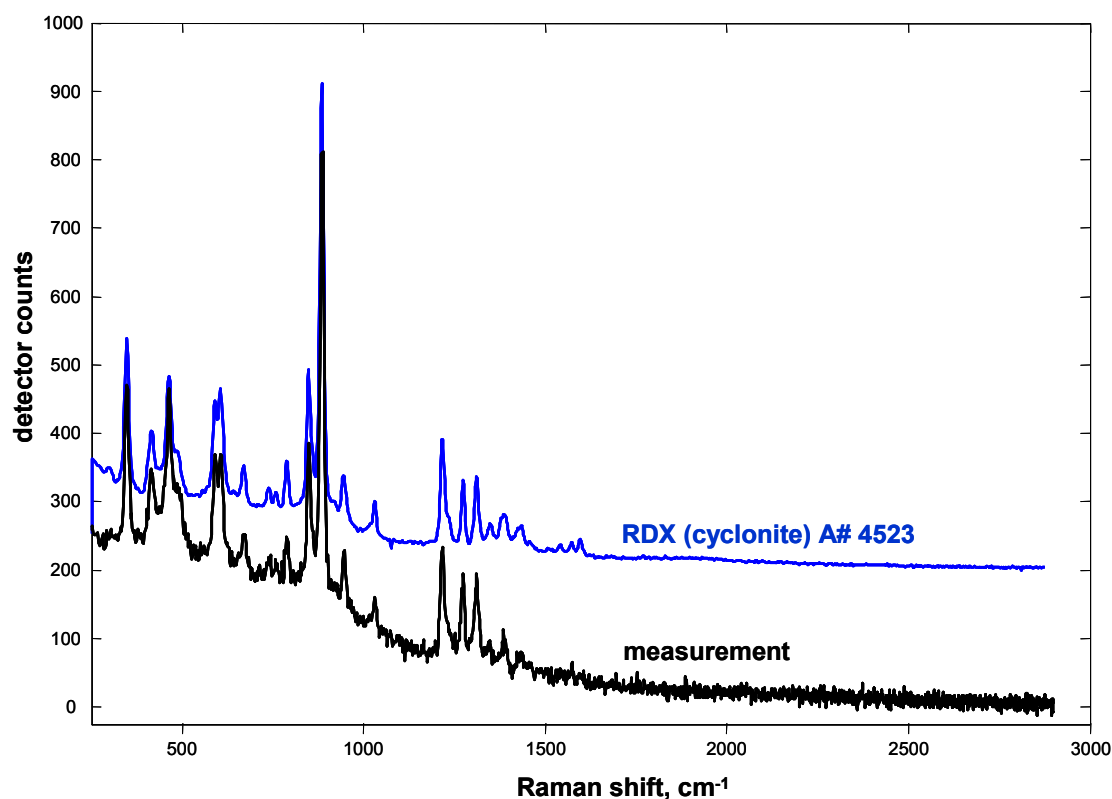
Figure 2.5. Spectral Overlay of Pure RDX (courtesy of Ahura Scientific) and a Field Forensic Sample Containing RDX

Analysis of the solid PETN sample resulted in a correct match to PETN in less than 30 seconds. Analysis of the 1000 ppm PETN/methanol mixture only identified methanol, further illustrating the challenge Raman spectroscopy has in identifying low concentrations in mixtures.

Analysis of Uncontained Material

Six substances were analyzed to determine how well the FirstDefender™ performed in analyzing an uncontained substance. Analyses for ammonium perchlorate, potassium nitrate, sodium bicarbonate, potassium chlorate and a commercial brand of corn starch produced correct matches but analyses of a commercial baby powder resulted in aborted scans. In previous experiments when the baby powder was in clear glass vials, the FirstDefender™ correctly matched the baby powder. Fluorescence was detected in all vial and point-and-shoot mode spectra involving the baby powder and likely overwhelmed any Raman signal generated in the analysis of uncontained baby powder. This illustrates a possible problem with field use of Raman spectroscopy and potential spectral complication due to motion; however, more research is required to assess this issue. In field practice, if no match or low probability matches are detected, stabilizing the unit at a fixed distance and re-scanning the substance should provide more precise data. A fiber optic probe attachment which is lighter and easier to stabilize may prove advantageous for field use.

CONCLUSION

The FirstDefender™ accurately identified many of the substances in vials when substances had corresponding library spectra. Of those substances, 83% were correctly or similarly matched in vial mode and 92% in point-and-shoot mode. This is especially noteworthy since most of the substances selected for this research are suspected to be problematic for measurement by Raman spectroscopy. White powder substances, which are prone to fluorescence, were generally identified correctly by the instrument. A very important finding was that no false positives were produced for substances present in the library.

When substances, without a corresponding spectra in the library, are analyzed, the preferred result would be no match found rather than an incorrect match (i.e. false positive) to a substance. Encouragingly, only 13% of both the vial and point-and-shoot analyses resulted in false positives. As the number of spectra in the library is increased, the number of false positive results is expected to decrease.

Thin transparent and translucent glass and plastic packaging materials had minimal effect on the accuracy of correct identification. Darker materials such as green glassware had a poorer signal-to-noise ratio. Substances such as hydrogen peroxide (3% in water) that produce weak Raman scatter could not be identified with the green glass containers. It was also observed that container markings such as volume markings on the vials interfered with accurate scans.

Binary liquid mixtures and explosive materials at concentrations 1% or less by volume proved difficult for the FirstDefender™. The instrument did identify ethanol in the 5% and 10% ethanol/water mixtures and generated a similar match to the 5% and

10% isopropanol (70% in water) and water mixtures but scans of all 1% mixtures were aborted. This finding supports observations from the literature that Raman is less reliable for identifying substances at low concentrations in mixtures. For example, PETN (> 99% purity) in powder form was correctly identified but was not identified in a 1000 ppm PETN/methanol mixture. It should be noted that if a mixture, such as jet fuel or gasoline, is loaded into the library, the mixture would more likely be identified.

Accurate and rapid detection with Raman spectrometry is enhanced with a large high quality spectral library. Approximately 80% of the library substances were correctly matched in vial and point-and-shoot scans. The percentage of correct matches should increase and the number of false positives should decrease as the number of library spectra increases.

As Raman spectrometry matures it should serve as a valuable screening tool to detect hazardous substances. Expanding the spectral library and continued improvements on algorithms to overcome fluorescence and materials with mild opacity will increase instrument accuracy. Proper training on instrument stability and focal point placement during field use is also important to generate a quality Raman signal.

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CHAPTER 3

CONCLUSION

Although this evaluation proved quite successful with no false positives identified for white powders, binary liquid mixtures in low concentrations proved challenging for the FirstDefender™. In the field, toxic chemicals could be masked within nontoxic materials and result in inaccurate detection especially if the masking agent is present in a high concentration and the toxic material in a low concentration.

The FirstDefender™ proved to be a reliable Raman spectrometer for rapidly identifying solid and liquid substances in clear, thin-walled containers (< 78 mils) provided the substance analyzed had a good corresponding library spectrum. This capability can be advantageous during forensic investigations or homeland security responses, when potentially hazardous materials are discovered inside containers and manual handling is not preferred to ensure first responder safety. The FirstDefender™ could be used at airport screening checkpoints to test suspicious liquids in clear containers.

Military personnel may be able to use the FirstDefender™ for identifying explosive materials or chemical warfare agents. However, care must be taken with dark materials that could overheat and ignite when using the laser at a 300 mW power setting. It is important to note that the FirstDefender™ cannot identify chemical warfare agents in the vapor phase. The FirstDefender™ could be used to identify contaminated areas where toxic chemicals spills have occurred by testing bulk materials on the ground.

Public Health Significance

Field-portable Raman spectrometers can be of tremendous value as a screening tool for public health personnel tasked with performing health risk assessments in an emergency response scenario. Using the FirstDefender™ in combination with other instruments can provide a more confident risk assessment. A toxicity assessment can be performed once public health personnel are reasonably certain that the hazard has been properly identified. Any associated risk to the general public and/or response personnel can then be disseminated.

Recommended Future Research

1. Binary Liquid Mixtures: Evaluate additional binary liquid mixtures to further evaluate the effectiveness of the instrument's mixture analysis capability. Additional research could explore how efficiently the instrument detects individual mixture components that are in the instrument library and correlate each component Raman cross-section to the percentage match for a mixture result.

2. Explosive Materials: Analyze liquid explosives and precursor materials in various clear plastic and glass containers.

3. Repeatability study with fiber-optic probe: Replicate this research with a handheld fiber-optic probe to determine probe effectiveness and repeatability of results.

4. Explore mathematical approaches to spectral deconvolution for improved search algorithms that compensate for fluorescence and sample heating.

APPENDIX A

FirstDefender™ Instrument Properties

Manufacturer	Ahura Scientific Corporation
Serial Number	FD1662
Mode of Operation	Automatic used for this research
Raman Shift Spectrum Range	250 cm^{-1} to 2875 cm^{-1}
Spectral Resolution	7 to 10 cm^{-1} (FWHM) across range
Laser Excitation	785 nm ± 0.5 nm, 3 cm^{-1} linewidth
Laser Power	300 mW used for this research
Detector	Silicon CCD 2048 pixels
Library Version	64
Number of Library Spectra	2151

APPENDIX B

Data Tables for All Experimental Phases

1. **Class: P = pure, C = commercial, B = biological**

2. **Physical: P = powder, L = liquid, S = solid, W = white, Y = yellow, O = orange, R = red, G = green, B = blue, Brn. = brown, Lt. = light, Clr. = colorless**

3. **Vial Mode**

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Ammonium dichromate	N	P	Y-O P	1	NMF
				2	NMF
				3	NMF
Ammonium perchlorate	Y	P	W P	1	Ammonium Perchlorate
				2	Ammonium Perchlorate
				3	Ammonium Perchlorate
Antimony oxalate	N	P	W P	1	NMF
				2	NMF
				3	NMF
Barium carbonate	Y	P	W P	1	66% Barium carbonate, 22.7% Potassium carbonate, 11.3% Magnesium nitrate hexahydrate
				2	75.6% Barium carbonate, 17.9% Potassium carbonate
				3	76.5% Barium carbonate, 17.4% Potassium carbonate

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Barium chlorate	N	P	W P	1	NMF
				2	NMF
				3	NMF
Barium nitrate	N	P	W P	1	91% Mixture: 59% Cluster of Silver nitrate, Ammonium bicarbonate, Ammonium carbonate…then 26% Trimethyl phosphate, 4% Potassium nitrate, 1% Mercury(I) nitrate dihydrate
				2	90% Mixture: 59% Cluster of Silver nitrate, Ammonium bicarbonate, Ammonium carbonate…then 26% Trimethyl phosphate, 4% Potassium nitrate, 2% Mercury(I) nitrate dihydrate
				3	90% Mixture: 60% Cluster of Silver nitrate, Ammonium bicarbonate, Ammonium carbonate…then 25% Trimethyl phosphate, 4% Potassium nitrate, 1% Mercury(I) nitrate dihydrate
Barium peroxide	Y	P	W P	1	Barium peroxide
				2	Barium peroxide
				3	Barium peroxide
Benzoic acid	Y	P	W P	1	Benzoic acid
				2	Benzoic acid
				3	Benzoic acid
Boric acid	N	P	W P	1	Mixture 82%: 75% Ethanol, 5% Potassium binoxalate, 2% Ethyl methylcarbamate
				2	Mixture 82%: 75% Ethanol, 6% Potassium binoxalate, 2% Ethyl methylcarbamate
				3	Mixture 82%: 75% Ethanol, 5% Potassium binoxalate, 2% Ethyl methylcarbamate
Calcium carbonate	Y	P	W P	1	58.9% Chalk, 41.1% Calcium carbonate
				2	58.8% Chalk, 41.2% Calcium carbonate
				3	59.5% Chalk, 40.5% Calcium carbonate
Cyclo hexane	Y	P	Clr. L	1	Cyclohexane
				2	Cyclohexane
				3	Cyclohexane
Hexamine	Y	P	W P	1	Hexamethylenetetramine
				2	Hexamethylenetetramine
				3	Hexamethylenetetramine

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Hydrogen peroxide 3%	Y	P	Clr. L	1	Hydrogen peroxide
				2	Hydrogen peroxide
				3	Hydrogen peroxide
Iron (III) oxide	N	P	R-O P	1	NMF
				2	Scan aborted; no result
				3	Scan aborted; no result
Isopropanol 70%	Y	P	Clr. L	1	2-Propanol
				2	2-Propanol
				3	2-Propanol
Lead nitrate	N	P	W P	1	Silver nitrate
				2	Silver nitrate
				3	Silver nitrate
Lead tetraoxide	N	P	O P	1	NMF
				2	NMF
				3	NMF
Magnesium carbonate	Y	P	W P	1	Magnesium carbonate hydroxide hydrate
				2	Magnesium carbonate hydroxide hydrate
				3	Magnesium carbonate hydroxide hydrate
Potassium chlorate	Y	P	W P	1	Potassium chlorate
				2	Potassium chlorate
				3	Potassium chlorate
Potassium nitrate	Y	P	W P	1	Potassium nitrate
				2	Potassium nitrate
				3	Potassium nitrate
Potassium perchlorate	Y	P	W P	1	Potassium perchlorate
				2	Potassium perchlorate
				3	Potassium perchlorate
Potassium sulfate	Y	P	W P	1	Potassium sulfate
				2	Potassium sulfate
				3	Mixture 96%: 90% Potassium sulfate, 6% Potassium carbonate

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
PVC powder	Y	P	W P	1	PVC
				2	PVC
				3	PVC
Sodium benzoate	Y	P	W P	1	Sodium benzoate
				2	Sodium benzoate
				3	Sodium benzoate
Sodium bicarbonate	Y	P	W P	1	Sodium bicarbonate
				2	Sodium bicarbonate
				3	Sodium bicarbonate
Sodium nitrate	Y	P	W P	1	Sodium nitrate
				2	Sodium nitrate
				3	Sodium nitrate
Sodium oxalate	Y	P	W P	1	Sodium oxalate
				2	Sodium oxalate
				3	Sodium oxalate
Sodium sulfate	Y	P	W P	1	45.3% Detergent, 44.0% Sodium sulfate, 5.7% Benzene
				2	44.0% Detergent, 42.6% Sodium sulfate, 7.5% 3-(Ethylamino)toluene
				3	47.8% Detergent, 47.6% Sodium sulfate
Strontium carbonate	N	P	W P	1	NMF
				2	NMF
				3	NMF
Strontium nitrate	N	P	W P	1	Mixture 79%: 56% Urea nitrate, 18% Thymol, 5% Cluster of Barium carbonate, Magnesium nitrate hexahydrate
				2	Mixture 77%: 54% Urea nitrate, 19% Thymol, 4% Cluster of Barium carbonate, Magnesium nitrate hexahydrate
				3	Mixture 77%: 53% Urea nitrate, 20% Thymol, 5% Cluster of Barium carbonate, Magnesium nitrate hexahydrate

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Strontium sulfate	N	P	W P	1	Mixture 71%: 41% trans, trans-2,3-Hexadienoic acid…24% Cluster of Benzyl alcohol, Benzyl acetate, Butylbenzene, Propylbenzene, Benzyl ether…4% Thioacetic acid, 2% Triphenyltin hydroxide
				2	Mixture 70%: 30% Cluster of Diphenylmethane, 1-Phenyldodecane, Mandelonitrile, 1-Phenyldecane, 1-Phenyltridecane, 1-Phenyltetradecane, 1-Phenylundecane…29% Resorcinol diglycidyl ether, 10% Sodium sulfide, 1% Triphenyltin hydroxide
				3	Mixture 70%: 38% Cluster of Diphenylmethane, 1-Phenyldodecane, Mandelonitrile, 1-Phenyldecane, 1-Phenyltridecane, 1-Phenyltetradecane, 1-Phenylundecane…20% Resorcinol diglycidyl ether, 12% Sodium sulfide
Baking powder	N	C	W P	1	NMF
				2	NMF
				3	Mixture 68%: 47% Calcium sulfate, 7% Plaster of Paris, 7% Cluster of Silver nitrate, Ammonium bicarbonate, Ammonium carbonate…5% 2-tert-Butylphenol
Bisquick	N	C	W P	1	35.6% Corn Meal (White), 35.2% Dextrin from corn, 29.2% Corn starch
				2	73% Mixture: 70% Cluster of Corn starch, Dextrin from corn, Corn Meal (White)…3% from something not listed
				3	Scan aborted; no result
Chlorowax	N	C	W P	1	Mixture 79%: 50% Bromine, 20% Antimony(v) chloride, 5% PVC, 4% Carbon tetrachloride
				2	Mixture 75%: 49% Bromine, 21% Antimony(v) chloride, 5% Carbon tetrachloride
				3	Mixture 78%: 48% Bromine, 21% Antimony(v) chloride, 6% PVC, 3% Carbon tetrachloride
Creamer, non-dairy (a)	N	C	W P	1	NMF
				2	NMF
				3	NMF

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Creamer, non-dairy (b)	N	C	W P	1	Mixture 91%: 63% Titanium(IV) oxide, anatase…23% Cluster of corn starch, Dextrin from corn, Corn Meal (white), 4% from something not listed, 1% 2-Ethoxyethyl acetate
				2	Mixture 90%: 62% Titanium(IV) oxide, anatase…25% Cluster of corn starch, Dextrin from corn, Corn Meal (white), 2% from something not listed, 1% 2-Ethoxyethyl acetate
				3	Mixture 89%: 63% Titanium(IV) oxide, anatase…25% Cluster of corn starch, Dextrin from corn, Corn Meal (white), 1% 2-Ethoxyethyl acetate
Detergent (a)	Y	C	W-B S-P	1	NMF
				2	NMF
				3	Scan aborted; no result
Equal	Y	C	W P	1	53.2% D-(+) Glucose, 46.8% alpha-D-Glucose
				2	55.0% D-(+) Glucose, 45.0% alpha-D-Glucose
				3	49.7% D-(+) Glucose, 50.3% alpha-D-Glucose
Gym chalk	Y	C	W P	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result
B. thuringiensis product	N	B	Brn S-P	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result
Saren Resin	N	C	W P	1	1.0% 2-Mercaptobenzothiazole sodium salt, 1.0% Formamide…a listing of many chemicals…all at 1.0%
				2	NMF
				3	NMF
Smoke Dye, yellow	N	C	Y P	1	NMF
				2	Scan aborted; no result
				3	NMF
Small Wonder Baby powder	Y	C	W P	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
VS Pear powder	Y	C	W P	1	NMF - sim cmpd...baby powder, foot powder
				2	NMF - sim cmpd...baby powder, foot powder
				3	NMF - sim cmpd...baby powder, foot powder
Corn starch	Y	B	W P	1	33.5% Corn starch, 33.4% Dextrin from corn, 33.0% Corn Meal (White)
				2	35.3% Corn starch, 32.7% Dextrin from corn, 32.1% Corn Meal (White)
				3	34.2% Corn starch, 35.6% Dextrin from corn, 30.2% Corn Meal (White)
Dextrin, corn	Y	B	W P	1	Corn starch
				2	45.5% Dextrin from corn, 28.9% Corn Meal (White), 25.6% Corn starch
				3	Scan aborted; no result
Flour, all-purpose	N	B	W P	1	35.8% Corn Meal (White), 32.6% Dextrin from corn, 31.6% Corn starch
				2	35.4% Corn Meal (White), 33.3% Dextrin from corn, 31.2% Corn starch
				3	37.9% Corn Meal (White), 33.3% Dextrin from corn, 28.1% Corn starch
Flour, rice	N	B	W P	1	35.0% Corn Meal (White), 33.3% Dextrin from corn, 31.5% Corn starch
				2	34.4% Corn Meal (White), 34.1% Dextrin from corn, 31.6% Corn starch
				3	34.8% Corn Meal (White), 31.5% Dextrin from corn, 33.6% Corn starch
Sugar, granulated	Y	B	W P	1	Sugar
				2	Sugar
				3	Sugar
Sugar, powdered	Y	B	W P	1	Sugar
				2	Sugar
				3	Sugar

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Detergent (a)	Y	C	W P	1	NMF
				2	Mixture 69%: 49% Sodium carbonate, 15% Cluster of Barium carbonate, Magnesium nitrate hexahydrate…3% Cluster of Sodium sulfate, Benzene, Detergent…3% Calcium peroxide hydrate
				3	NMF
Formic Acid 90%	Y	P	Clr. L	1	Formic acid
				2	Formic acid
				3	Formic acid
Glacial Acetic Acid	Y	P	Clr. L	1	Acetic acid
				2	Acetic acid
				3	Acetic acid
Ammonium hydroxide	N	P	Clr. L	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result
Sodium hydroxide	N	P	Clr. L	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result
DMMP	Y	P	Clr. L	1	Dimethyl methylphosphonate
				2	Dimethyl methylphosphonate
				3	Dimethyl methylphosphonate
DIMP	N	P	Clr. L	1	GB (sarin nerve agent)
				2	GB (sarin nerve agent)
				3	GB (sarin nerve agent)
Oxalic acid	Y	P	Brn. P	1	NMF
				2	NMF
				3	NMF

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
J&J Baby Powder	Y	C	W P	1	62.2% Baby powder, 35.2% foot powder
				2	63.6% Baby powder, 33.3% foot powder
				3	67.3% Baby powder, 31.5% foot powder
Ammonium nitrate	Y	P	W S-P	1	89.1% Ammonium nitrate, 7.1% Silver nitrate
				2	Ammonium nitrate
				3	Ammonium nitrate

4. Point-and-Shoot Mode

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Ammonium dichromate	N	P	Y-O P	1	NMF
				2	NMF
				3	NMF
Ammonium perchlorate	Y	P	W P	1	Ammonium perchlorate
				2	Ammonium perchlorate
				3	Ammonium perchlorate
Antimony oxalate	N	P	W P	1	NMF
				2	NMF
				3	NMF
Barium carbonate	Y	P	W P	1	71.5% Barium carbonate, 17.6% Potassium carbonate, 10.9% Magnesium nitrate hexahydrate
				2	74.8% Barium carbonate, 18.6% Potassium carbonate
				3	65.8% Barium carbonate, 22.5% Potassium carbonate, 11.7% Magnesium nitrate hexahydrate
Barium chlorate	N	P	W P	1	NMF
				2	NMF
				3	NMF

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Barium nitrate	N	P	W P	1	Mixture 90%: 59% Cluster of Silver nitrate, Ammonium bicarbonate, Ammonium carbonate…26% Trimethyl phosphate, 4% Potassium nitrate, 1% Mercury(I) nitrate dihydrate
				2	Mixture 91%: 58% Cluster of Silver nitrate, Ammonium bicarbonate, Ammonium carbonate…28% Trimethyl phosphate, 4% Potassium nitrate, 2% Mercury(I) nitrate dihydrate
				3	Mixture 91%: 59% Cluster of Silver nitrate, Ammonium bicarbonate, Ammonium carbonate…27% Trimethyl phosphate, 4% Potassium nitrate, 2% Mercury(I) nitrate dihydrate
Barium peroxide	Y	P	W P	1	Barium peroxide
				2	Barium peroxide
				3	Barium peroxide
Benzoic acid	Y	P	W P	1	Benzoic acid
				2	Benzoic acid
				3	Benzoic acid
Boric acid	N	P	W P	1	Mixture 82%: 75% Ethanol, 6% Potassium binoxalate, 1% Calcium chromate
				2	Mixture 81%: 75% Ethanol, 5% Potassium binoxalate, 1% Calcium chromate
				3	Mixture 80%: 75% Ethanol, 5% Potassium binoxalate
Calcium carbonate	Y	P	W P	1	61.9% Chalk, 38.1% Calcium carbonate
				2	Chalk
				3	65.5% Chalk, 34.5% Calcium carbonate
Cyclo hexane	Y	P	Clr. L	1	Cyclohexane
				2	Cyclohexane
				3	Cyclohexane
Hexamine	Y	P	W P	1	Hexamethylenetetramine
				2	Hexamethylenetetramine
				3	Hexamethylenetetramine

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Hydrogen peroxide 3%	Y	P	Clr. L	1	Hydrogen peroxide
				2	Hydrogen peroxide
				3	Hydrogen peroxide
Iron (III) oxide	N	P	R-O P	1	Scan aborted; no result
				2	Scanning error; auto exposure failed…try lowering laser power
				3	Scan aborted; no result
				4	Scanning error; auto exposure failed…try lowering laser power
Isopropanol 70%	Y	P	Clr. L	1	2-Propanol
				2	2-Propanol
				3	2-Propanol
Lead nitrate	N	P	W P	1	Silver nitrate
				2	89.2% Silver nitrate, 9.4% Mercury(I) nitrate dihydrate
				3	84.2% Silver nitrate, 12.1% Mercury(I) nitrate dihydrate
Lead tetraoxide	N	P	O P	1	NMF
				2	NMF
				3	NMF
Magnesium carbonate	Y	P	W P	1	Mixture 94%: 89% Magnesium carbonate hydroxide hydrate, 6% Missing(?)
				2	Mixture 93%: 84% Magnesium carbonate hydroxide hydrate, 8% Missing(?), 1% Silicon tetrachloride
				3	Scan aborted; no result
				4	Mixture 93%: 60% Magnesium carbonate hydroxide hydrate, 32% Missing(?), Sillicon tetrachloride 1%
Potassium chlorate	Y	P	W P	1	Potassium chlorate
				2	Potassium chlorate
				3	Potassium chlorate
Potassium nitrate	Y	P	W P	1	Potassium nitrate
				2	Potassium nitrate
				3	Potassium nitrate

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Potassium perchlorate	Y	P	W P	1	Potassium perchlorate
				2	Potassium perchlorate
				3	Potassium perchlorate
Potassium sulfate	Y	P	W P	1	Potassium sulfate
				2	Potassium sulfate
				3	Potassium sulfate
PVC powder	Y	P	W P	1	PVC
				2	Scan aborted; no result
				3	PVC
Sodium benzoate	Y	P	W P	1	Sodium benzoate
				2	Sodium benzoate
				3	Sodium benzoate
Sodium bicarbonate	Y	P	W P	1	Sodium bicarbonate
				2	Sodium bicarbonate
				3	Sodium bicarbonate
Sodium carbonate	Y	P	W P	1	NMF
				2	Mixture 78%: 52% Sodium nitrate, 21% Potassium carbonate, 4% Diethanolamine lauryl sulfate, 2% Methamidophos
				3	NMF
				4	NMF
Sodium nitrate	Y	P	W P	1	Sodium nitrate
				2	Sodium nitrate
				3	Sodium nitrate
Sodium oxalate	Y	P	W P	1	Sodium oxalate
				2	Sodium oxalate
				3	Sodium oxalate

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Sodium sulfate	Y	P	W P	1	54.6% Sodium sulfate, 45.4% Detergent
				2	48.3% Sodium sulfate, 48.6% Detergent
				3	50.8% Sodium sulfate, 48.7% Detergent
Strontium carbonate	N	P	W P	1	NMF
				2	NMF
				3	NMF
Strontium nitrate	N	P	W P	1	Mixture 84%: 54% Thymol, 20% Sulfamic acid, 5% Urea nitrate, 5% Cluster of Barium carbonate, Magnesium nitrate hexahydrate
				2	Mixture 80%: 53% Cluster of Barium carbonate, Magnesium nitrate hexahydrate…16% o-Xylene, 9% Urea nitrate, 1% Potassium nitrate
				3	Mixture 80%: 55% Cluster of Barium carbonate, Magnesium nitrate hexahydrate…15% o-Xylene, 9% Urea nitrate, 1% Potassium nitrate
Strontium sulfate	N	P	W P	1	NMF…sim match Hydroxylamine hydrochloride
				2	NMF…sim match Hydroxylamine hydrochloride
				3	NMF…sim match Hydroxylamine hydrochloride
				4	Mixture 87%: 70% trans, trans-2,4-Hexandienoic acid potassium salt, 13% Sodium sulfide, 3% Resorcinol diglycidyl ether, 1% Thioacetic acid
				5	Mixture 81%: 70% trans, trans-2,4-Hexandienoic acid potassium salt, 9% Sodium sulfide, 2% Resorcinol diglycidyl ether
Baking powder	N	C	W P	1	NMF
				2	NMF
				3	NMF
				4	NMF…sim match to Calcium sulfate
				5	NMF
Bisquick	N	C	W P	1	39% Corn Meal (White), 32.6% Dextrin from corn, 28.1% Corn starch
				2	Scan aborted; no result
				3	Scan aborted; no result
				4	Mixture 76%: 67% Cluster of Corn starch, Dextrin from corn, Corn Meal (White)…9% Missing
				5	Mixture 85%: 59% Missing, 67% Cluster of Corn starch, Dextrin from corn, Corn Meal (White)

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Chlorowax	N	C	W P	1	Mixture 79%: 48% Bromine, 21% Antimony(v) chloride, 5% PVC, 4% Carbon tetrachloride
				2	Mixture 79%: 49% Bromine, 20% Antimony(v) chloride, 7% PVC, 3% Carbon tetrachloride
				3	Mixture 79%: 49% Bromine, 21% Antimony(v) chloride, 5% PVC, 4% Carbon tetrachloride
				4	Mixture 83%: 49% Bromine, 29% Soda lime, 4% Missing, 1% Carbon tetrachloride
Creamer, non-dairy (a)	N	C	W P	1	NMF
				2	Scan aborted; no result
				3	Scan aborted; no result
				4	NMF
Creamer, non-dairy (b)	N	C	W P	1	Mixture 86%: 63% Titanium(IV) oxide, anatase…24% Cluster of Corn starch, Dextrin from corn, Corn Meal (White)
				2	NMF
				3	Mixture 87%: 64% Titanium(IV) oxide, anatase…22% Cluster of Corn starch, Dextrin from corn, Corn Meal (White)
Detergent (a)	Y	C	W-B S-P	1	NMF
				2	Scan aborted; no result
				3	Scan aborted; no result
				4	NMF
Equal	Y	C	W P	1	58.5% D-(+) Glucose, 41.5% alpha-D-Glucose
				2	57.2% D-(+) Glucose, 42.8% alpha-D-Glucose
				3	56.5% D-(+) Glucose, 43.5% alpha-D-Glucose
				4	56.0% D-(+) Glucose, 44.0% alpha-D-Glucose
Gym chalk	Y	C	W P	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result
				4	Mixture 87%: 55% Missing, 28% Magnesium carbonate hydroxide hydrate, 4% Silicon tetrachloride
				5	Mixture 69%: 33% Missing, 33% Magnesium carbonate hydroxide hydrate, 3% Silicon tetrachloride

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
B. thuringiensis product	N	B	Brn S-P	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result
Saren Resin	N	C	W P	1	NMF
				2	NMF
				3	NMF
				4	NMF
Smoke Dye, yellow	N	C	Y P	1	NMF
				2	NMF
				3	NMF
				4	NMF
Small Wonder Baby powder	Y	C	W P	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result
VS Pear powder	Y	C	W P	1	Scan aborted; no result
				2	71.4% Baby powder, 27.5% Foot powder
				3	68.3% Baby powder, 30.3% Foot powder
Corn starch	Y	B	W P	1	35.7% Corn starch, 32.3% Corn Meal (White), 31.9% Dextrin from corn
				2	36.9% Corn starch, 31.7% Corn Meal (White), 31.4% Dextrin from corn
				3	35.1% Corn starch, 32.6% Corn Meal (White), 32.3% Dextrin from corn
Dextrin, corn	Y	B	W P	1	Scan aborted; no result
				2	NMF…sim match to Dextrin from corn, Corn Meal (White), Corn starch
				3	43.5% Dextrin from corn, 28.5% Corn Meal (White), 28.0% Corn starch

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Flour, all-purpose	N	B	W P	1	34.7% Corn Meal (White), 34.4% Dextrin from corn, 30.8% Corn starch
				2	37.1% Corn Meal (White), 32.6% Dextrin from corn, 30.3% Corn starch
				3	39.7% Corn Meal (White), 31.8% Dextrin from corn, 28.5% Corn starch
Flour, rice	N	B	W P	1	34.4% Corn Meal (White), 32.2% Dextrin from corn, 33.3% Corn starch
				2	39.2% Corn Meal (White), 28.7% Dextrin from corn, 32.0% Corn starch
				3	37.9% Corn Meal (White), 29.9% Dextrin from corn, 32.2% Corn starch
Sugar, granulated	Y	B	W P	1	Sugar
				2	Sugar
				3	Sugar
Sugar, powdered	Y	B	W P	1	Sugar
				2	Sugar
				3	Sugar
Detergent (b)	Y	C	W P	1	Mixture 95%: 92% Sodium carbonate, 3% Cluster of Sodium sulfate, Benzene, Detergent
				2	Mixture 92%: 85% Sodium carbonate, 5% Cluster of Sodium sulfate, Benzene, Detergent…2% Missing
				3	Mixture 93%: 86% Sodium carbonate, 3% Sodium n-hexadecyl sulphate, 2% Resorcinol diglycidyl ether, 2% Missing
Formic Acid 90%	Y	P	Clr. L	1	Formic Acid
				2	Formic Acid
				3	Formic Acid
Glacial Acetic Acid	Y	P	Clr. L	1	Acetic acid
				2	Acetic acid
				3	Acetic acid
Ammonium hydroxide	N	P	Clr. L	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result

Compound	In Library	Class	Physical	Scan	Result from FirstDefender
Sodium hydroxide	N	P	Clr. L	1	Scan aborted; no result
				2	Scan aborted; no result
				3	Scan aborted; no result
DMMP	Y	P	Clr. L	1	Dimethyl methylphosphonate
				2	Dimethyl methylphosphonate
				3	Dimethyl methylphosphonate
DIMP	N	P	Clr. L	1	GB (sarin nerve agent)
				2	GB (sarin nerve agent)
				3	GB (sarin nerve agent)
Oxalic acid	Y	P	Brn. P	1	NMF
				2	NMF
				3	Scan aborted; no result
J&J Baby Powder	Y	C	W P	1	69.3% Baby powder, 28.5% Foot powder
				2	66.4% Baby powder, 31.5% Foot powder
				3	68.7% Baby powder, 30.0% Foot powder
Ammonium nitrate	Y	P	W S-P	1	Ammonium nitrate
				2	Ammonium nitrate
				3	Ammonium nitrate
				4	Ammonium nitrate

5. Packaging Material and Container Effects

Container	Compound	Physical	Scan	Results
50 mL BD Falcon tube	3% Hydrogen peroxide	Clr. L	1	Mixture 80%: 77% Hydrogen peroxide, 3% Barium peroxide
			2	Mixture 95%: 82% Hydrogen peroxide, 13% Polypropylene
			3	Scan aborted; no result
			4	Mixture 79%: 74% Hydrogen peroxide, 4% Barium peroxide, 1% 3,5-Dichlorophenol
	Isopropanol 70%	Clr. L	1	84.7% 2-Propanol, 14.9% Expo2 White Board Cleaner
			2	89.9% 2-Propanol, 9.9% Expo2 White Board Cleaner
			3	87.8% 2-Propanol, 11.7% Expo2 White Board Cleaner
	Ammonium perchlorate	W P	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Mixture 97%: 93% Ammonium perchlorate, 4% Polypropylene
	Potassium nitrate	W P	1	Potassium nitrate
			2	Potassium nitrate
			3	Mixture 94%: 93% Potassium nitrate, 1% Barium peroxide

Container	Compound	Physical	Scan	Results
15 mL BD Falcon tube	3% Hydrogen peroxide	Clr. L	1	Mixture 95%: 57% Hydrogen peroxide, 38% Cluster of Polystyrene, Ethyl 3-methyl-3-phenylglycidate
			2	Mixture 91%: 13% Hydrogen peroxide, 77% Cluster of Polystyrene, Ethyl 3-methyl-3-3phenylglycidate…1% Cluster of Benzyl Alcohol, Benzyl Acetate, Butylbenzene, Propylbenzene, Benzyl ether
			3	Mixture 95%: 59% Hydrogen peroxide, 37% Cluster of Polystyrene, Ethyl 3-methyl-3-phenylglycidate
	Isopropanol 70%	Clr. L	1	89.5% 2-Propanol, 10.3% Expo2 White Board Cleaner
			2	86.3% 2-Propanol, 13.6% Expo2 White Board Cleaner
			3	86.5% 2-Propanol, 13.0% Expo2 White Board Cleaner
	Ammonium perchlorate	W P	1	Mixture 97%: 93% Ammonium perchlorate, 3% Cluster of 3-Phenoxybenzyl alcohol, 3-Phenoxybenzaldehyde, Hydroxylamine hydrochloride, Permethrin
			2	Mixture 96%: 93% Ammonium perchlorate, 3% Cluster of 3-Phenoxybenzyl alcohol, 3-Phenoxybenzaldehyde, Hydroxylamine hydrochloride, Permethrin
			3	Mixture 73%: 38% Tetraethylammonium perchlorate, 32% Cluster of Diphenylmethane, 1-Phenyldodecane, mandelonitrile, 1-Phenyldecane, 1-Phenyltridecane, 1-Phenyltetradecane, 1-Phenylundecane…3% (R)-(-)-Phenyldephrine hydrochloride
	Potassium nitrate	W P	1	Mixture 98%: 91% Potassium nitrate, 8% Cluster of Benzyl alcohol, Benzyl acetate, Butlybenzene, Propylbenzene, Benzyl ether
			2	Mixture 98%: 94% Potassium nitrate, 4% Cluster of 3-Phenoxybenzyl alcohol, 3-Phenoxybenzaaldehyde, Hydroxylamine hydrochloride, Permethrin
			3	Mixture 94%: 21% Potassium nitrate, 72% Cluster of 3-Phenoxybenzyl alcohol, 3-Phenoxybenzaaldehyde, Hydroxylamine hydrochloride, Permethrin

Container	Compound	Physical	Scan	Results
1.2 mL Corning Cryovial *Polypropylene*	3% Hydrogen peroxide	Clr. L	1	Polypropylene
			2	Scan aborted; no result
			3	Polypropylene
			4	Mixture 73%: 68% Polypropylene, 5% 2-(isopropylamino)ethanol
	Isopropanol 70%	Clr. L	1	NMF…sim match to 2-Propanol, Expo2 White Board Cleaner, Trifluroroacetic acid
			2	Mixture 92%: 90% 2-Propanol, 2% Expo2 White Board Cleaner
			3	2-Propanol
	Ammonium perchlorate	W P	1	Ammonium perchlorate
			2	Mixture 93%: 52% Polypropylene, 41% Ammonium perchlorate
			3	Ammonium perchlorate
			4	Scan aborted; no result
	Potassium nitrate	W P	1	Potassium nitrate
			2	Mixture 98%: 89% Potassium nitrate, 9% Polypropylene
			3	NMF
500 mL PE container	3% Hydrogen peroxide	Clr. L	1	Mixture 89%: 79% Hydrogen peroxide, 10% Dioctyl terephthalate
			2	Mixture 87%: 64% Hydrogen peroxide, 21% Dioctyl terephthalate, 3% Hexamethylphosphoramide
			3	Mixture 88%: 66% Hydrogen peroxide, 19% Dioctyl terephthalate, 3% Hexamethylphosphoramide
	Isopropanol 70%	Clr. L	1	83.8% 2-Propanol, 15.9% Expo2 White Board Cleaner
			2	2-Propanol
			3	2-Propanol
Green Glass Soda Bottle	3% Hydrogen peroxide	Clr. L	1	Scan aborted; no result
			2	Scan aborted; no result
			3	Scan aborted; no result
	Isopropanol 70%	Clr. L	1	NMF…sim match to 2-Propanol, Expo2 White Board Cleaner
			2	82.5% 2-Propanol, 17.1% Expo2 White Board Cleaner
			3	2-Propanol

Container	Compound	Physical	Scan	Results
2 mL Amber Glass Vials	3% Hydrogen peroxide	Clr. L	1	Hydrogen peroxide
			2	Scan aborted; no result
			3	Hydrogen peroxide
	Isopropanol 70%	Clr. L	1	2-Propanol
			2	2-Propanol
			3	2-Propanol
Green Wine Bottle	3% Hydrogen peroxide	Clr. L	1	Scan aborted; no result
			2	Scan aborted; no result
			3	Scan aborted; no result
	Isopropanol 70%	Clr. L	1	82.3% 2-Propanol, 13.9% Expo2 White Board Cleaner
			2	84.8% 2-Propanol, 14.7% Expo2 White Board Cleaner
			3	79.1% 2-Propanol, 18.6% Expo2 White Board Cleaner
Kapak bag	Ammonium perchlorate	W P	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
	Potassium nitrate	W P	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
	Sodium bicarbonate	W P	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
	Potassium chlorate	W P	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate

Container	Compound	Physical	Scan	Results
Aloksak	Ammonium perchlorate	W P	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
	Potassium nitrate	W P	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
	Sodium bicarbonate	W P	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
	Potassium chlorate	W P	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate
Bitran bag	Ammonium perchlorate	W P	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
	Potassium nitrate	W P	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
	Sodium bicarbonate	W P	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
	Potassium chlorate	W P	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate

6. Influence of Material Thickness

Material	Compound	Thickness mils	Scan	Results
Kapak bag	Ammonium perchlorate	13.5000	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
		22.5000	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
		31.5000	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
		58.5000	1	NMF…sim match to Ammonium perchlorate
			2	NMF…sim match to Ammonium perchlorate, Potassium perchlorate
			3	NMF…sim match to Ammonium perchlorate
		76.5000	1	Mixture 84%: 67% Ammonium perchlorate, 11% Didocecyl 3,3'-thiodipropionate, 4% Nylon, 3% Ethylene glycol diacetate
			2	Mixture 85%: 83% Ammonium perchlorate, 2% Cluster of Barium carbonate, Magnesium nitrate hexahydrate
			3	Mixture 89%: 84% Ammonium perchlorate, 4% Nylon, 1% Ethylene glycol diacetate
Kapak bag	Potassium nitrate	13.5000	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
		22.5000	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate

Material	Compound	Thickness mils	Scan	Results
Kapak bag	Potassium nitrate	31.5000	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
		58.5000	1	Mixture 92%: 91% Potassium nitrate, 1% Ethylene glycol diacetate
			2	NMF…sim match to Potassium nitrate
			3	NMF…sim match to Potassium nitrate
		76.5000	1	NMF
			2	Mixture 70%: 68% Potassium nitrate, 2% Strontium peroxide
			3	Mixture 90%: 69% Potassium nitrate, 12% Octadecanamide, 10% Polyethylene terephthalate
Kapak bag	Sodium bicarbonate	13.5000	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
		22.5000	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
		31.5000	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
		58.5000	1	Mixture 71%: 66% Sodium bicarbonate, 3% Dimetilan, 1% Dioctyl terephthalate
			2	NMF
			3	NMF
		76.5000	1	NMF
			2	Scan aborted; no result
			3	Scan aborted; no result
Kapak bag	Potassium chlorate	13.5000	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate

Material	Compound	Thickness mils	Scan	Results
Kapak bag	Potassium chlorate	22.5000	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate
		31.5000	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate
		58.5000	1	92% Mixture: 79% Potassium chlorate, 10% Cluster of HDPE, HDPE-UV, Low density polyethylene, Vybar Wax Additives, Beeswax…1% Cluster of Lead (II) perchlorate trihydrate, Perchloric acid…1% Strontium peroxide
			2	90% Mixture: 81% Potassium chlorate, 7% Didodecyl 3,3'-thiodipropionate, 1% Sodium chlorate, 1% Nylon
			3	90% Mixture: 79 % Potassium chlorate, 8% Didodecyl 3,3'-thiodipropionate, 1% Sodium chlorate, 1% Nylon
		76.5000	1	NMF
			2	Scan aborted; no result
			3	NMF
Aloksak	Ammonium perchlorate	18.0000	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
		30.0000	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
		42.0000	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
		78.0000	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate

Material	Compound	Thickness mils	Scan	Results
Aloksak	Ammonium perchlorate	114.0000	1	Ammonium perchlorate
			2	Ammonium perchlorate
			3	Ammonium perchlorate
Aloksak	Potassium nitrate	18.0000	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
		30.0000	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
		42.0000	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
		78.0000	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
		114.0000	1	Potassium nitrate
			2	Potassium nitrate
			3	Potassium nitrate
Aloksak	Sodium bicarbonate	18.0000	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
		30.0000	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
		42.0000	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate

Material	Compound	Thickness mils	Scan	Results
Aloksak	Sodium bicarbonate	78.0000	1	Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
		114.0000	1	NMF…sim match to Sodium bicarbonate
			2	Sodium bicarbonate
			3	Sodium bicarbonate
Aloksak	Potassium chlorate	18.0000	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate
		30.0000	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate
		42.0000	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate
		78.0000	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate
		114.0000	1	Potassium chlorate
			2	Potassium chlorate
			3	Potassium chlorate

7. Influence of Chemical Concentration

Compound	Conc/Solvent	Scan	Results
Isopropyl alcohol 70% in water	10%/H2O	1	73.2% Expo2 White Board Cleaner, 23.1% 2-Propanol
		2	69.3% Expo2 White Board Cleaner, 23.8% 2-Propanol
		3	78% Expo2 White Board Cleaner, 20.5% 2-Propanol
	5%/H2O	1	73.6% Expo2 White Board Cleaner, 21.8% 2-Propanol
		2	81.9% Expo2 White Board Cleaner, 16.5% 2-Propanol
		3	67.0% Expo2 White Board Cleaner, 28.5% 2-Propanol
	1%/H2O	1	Scan aborted; no result
		2	Scan aborted; no result
		3	Scan aborted; no result
Ethanol	10%/H2O	1	86% Mixture: 79% Ethanol, 5% Ethylamine, 1% Missing
		2	76.6% Ethanol, 16.3% Ethylamine
		3	96% Mixture: 66% Missing, 28% Ethanol, 2% Chewing gum, sugarless
	5%/H2O	1	80% Mixture: 58% Hydrogen peroxide, 21% Missing, 2% Ethanol
		2	76% Mixture: 71% Missing, 4% Ethylamine, 1% Ethanol
		3	77% Mixture: 77% Ethanol, 4% Ethylamine, 4% Missing
	1%/H2O	1	Scan aborted; no result
		2	Scan aborted; no result
		3	Scan aborted; no result
DMMP	10%/H2O	1	81.1% Bleach, regular…18.3% Dimethyl methylphosphonate
		2	85% Mixture: 81% Bleach, regular….4% 2-Bromo-2-chloro-1,1,1-trifluoroethane
		3	90% Misture: 53% Thioacetamide, 34% Bleach, regular…2% Dimethyl methylphosphonate, 1% 2-Bromo-2-chloro-1,1,1-trifluoroethane
	5%/H2O	1	96% Mixture: 84% Missing, 7% Dimethyl methylphosphonate, 6% Thioacetamide
		2	77.5% Bleach, regular…21.2% Dimethyl methylphosphonate
		3	88% Mixture: 71% Missing, 14% Bleach, regular….3% 2-Bromo-2-chloro-1,1,1-trifluoroethane
	1%/H2O	1	Scan aborted; no result
		2	Scan aborted; no result
		3	Scan aborted; no result

8. Explosive Materials

Compound	Scan	Results
PETN	1	PETN
	2	PETN
PETN	1	Methanol
1000 ppm in methanol	2	Methanol
RDX field sample 1	1	NMF
	2	Scan aborted; no result
	3	NMF
RDX field sample 2	1	NMF
	2	NMF
	3	NMF, sim match to RDX
	4	NMF
RDX field sample 3	1	NMF
	2	NMF
	3	NMF
RDX field sample 4	1	NMF
	2	NMF
	3	NMF
RDX field sample 5	1	NMF
	2	NMF
	3	NMF

Compound	Scan	Results
RDX field sample 6	1	NMF
	2	NMF
	3	NMF
RDX field sample 7	1	Mixture 71%: 63% RDX (cyclonite), 5% Propyl formate, 2% 2-Octanol
	2	NMF
	3	NMF
RDX field sample 8	1	NMF
	2	Mixture 74%: 63% RDX (cyclonite), 9% 2,3-Dimethyloxirane, 2% 2-Octanol
	3	NMF
RDX field sample 9	1	NMF
	2	NMF
	3	NMF
RDX field sample 10	1	NMF
	2	NMF
	3	Scan aborted; no result
RDX field sample 11	1	Scan aborted; no result
RDX field sample 12	1	NMF
	2	NMF
	3	NMF
RDX field sample 13	1	NMF
	2	NMF
	3	NMF

9. Uncontained Material

Compound	Scan	Results
Ammonium perchlorate	1	Ammonium perchlorate
	2	Ammonium perchlorate
	3	Ammonium perchlorate
Potassium nitrate	1	Potassium nitrate
	2	Potassium nitrate
	3	Potassium nitrate
Sodium bicarbonate	1	NMF, sim match to Sodium bicarbonate
	2	Sodium bicarbonate
	3	Sodium bicarbonate
Potassium chlorate	1	Potassium chlorate
	2	Potassium chlorate
	3	Potassium chlorate
J&J Baby Powder	1	Scan aborted; no result
	2	Scan aborted; no result
	3	Scan aborted; no result
Corn Starch	1	34.1% Corn starch, 31.9% Dextrin from corn, 33.9% Corn Meal (White)
	2	NMF
	3	24.6% Corn starch, 28.4% Dextrin from corn, 47.0% Corn Meal (White)

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Capt Joseph L. Catyb graduated from Rensselaer Polytechnic Institute in 1994 with a Bachelor of Science in Civil Engineering and a concentration in Environmental Engineering. He served as the Deputy Chief, Bioenvironmental Engineering at Pope AFB from 1999-2002 where he supported air mobility operations for over 120 industrial workplaces and managed the base environmental health program. While stationed at Kunsan AB from 2002-2003 he served as Deputy Chief, Bioenvironmental Engineering, managing both the Industrial Hygiene and Environmental Health Programs and was the 8th Medical Operations Squadron Company Grade Officer of 2002. From 2003-2005, he served as Chief, Bioenvironmental Engineering Command Core System at Brooks AFB. In 2005, he entered the Graduate School of Uniformed Services University in the Public Health and Biometrics Department. Upon graduation in June 2007, he will be assigned as the Flight Commander for Bioenvironmental Engineering at Beale AFB.